Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# *Supporting Information*

## *Halogen atom effect of fluorinated tolanes on their luminescence characteristics*

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## Contents

## 1. $^{1}$H-, $^{19}$F-, $^{13}$C-NMR, and IR spectra

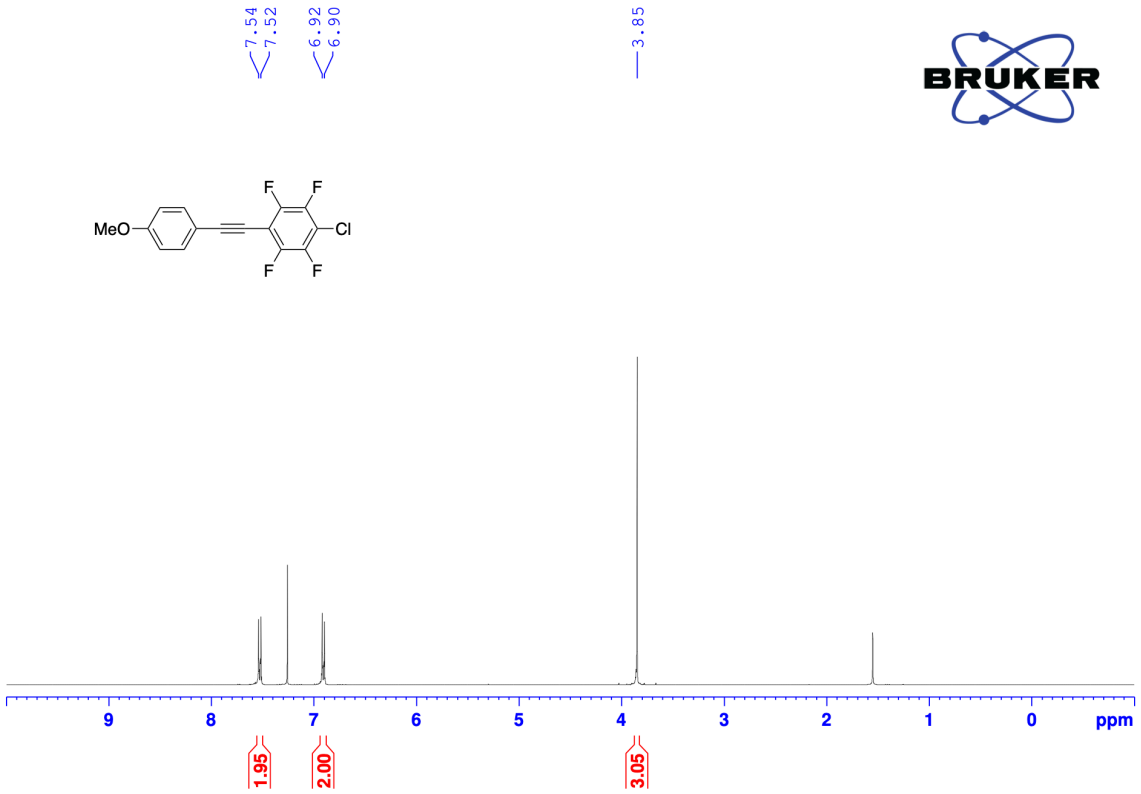



**Figure S1** $^{1}$H NMR spectrum of **4F-Cl**.

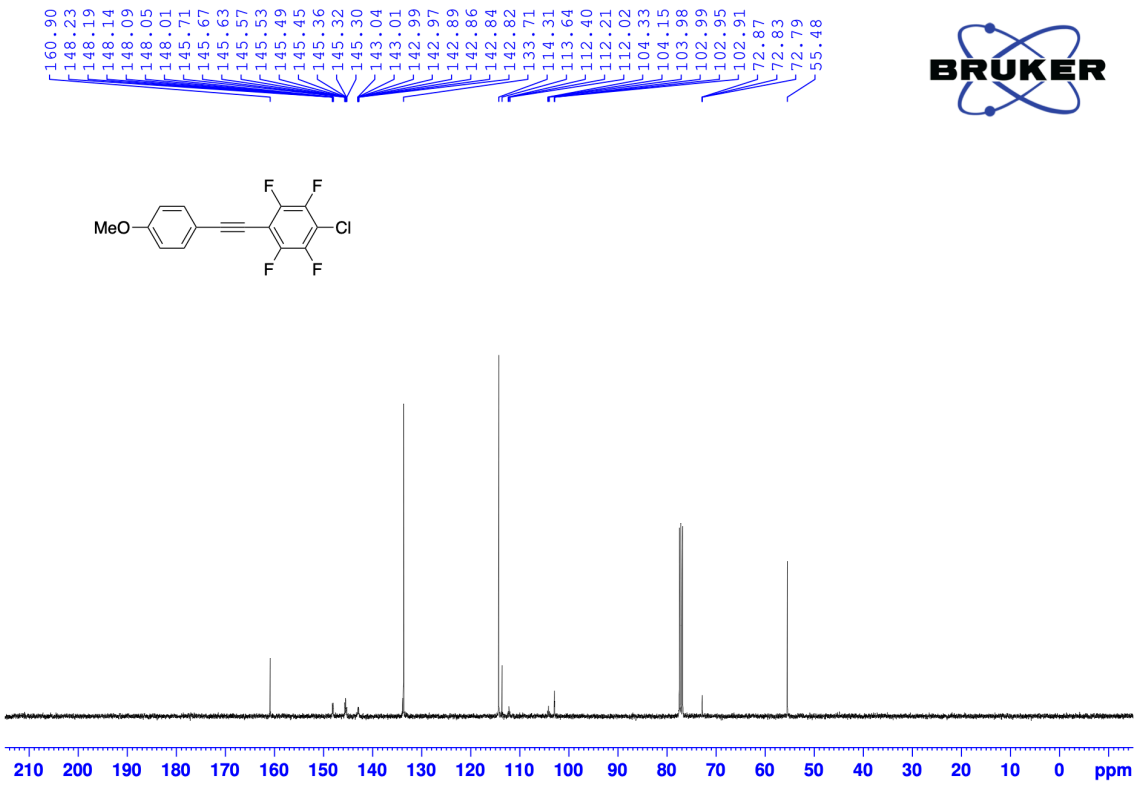



**Figure S2** $^{13}$C NMR spectrum of **4F-Cl**.

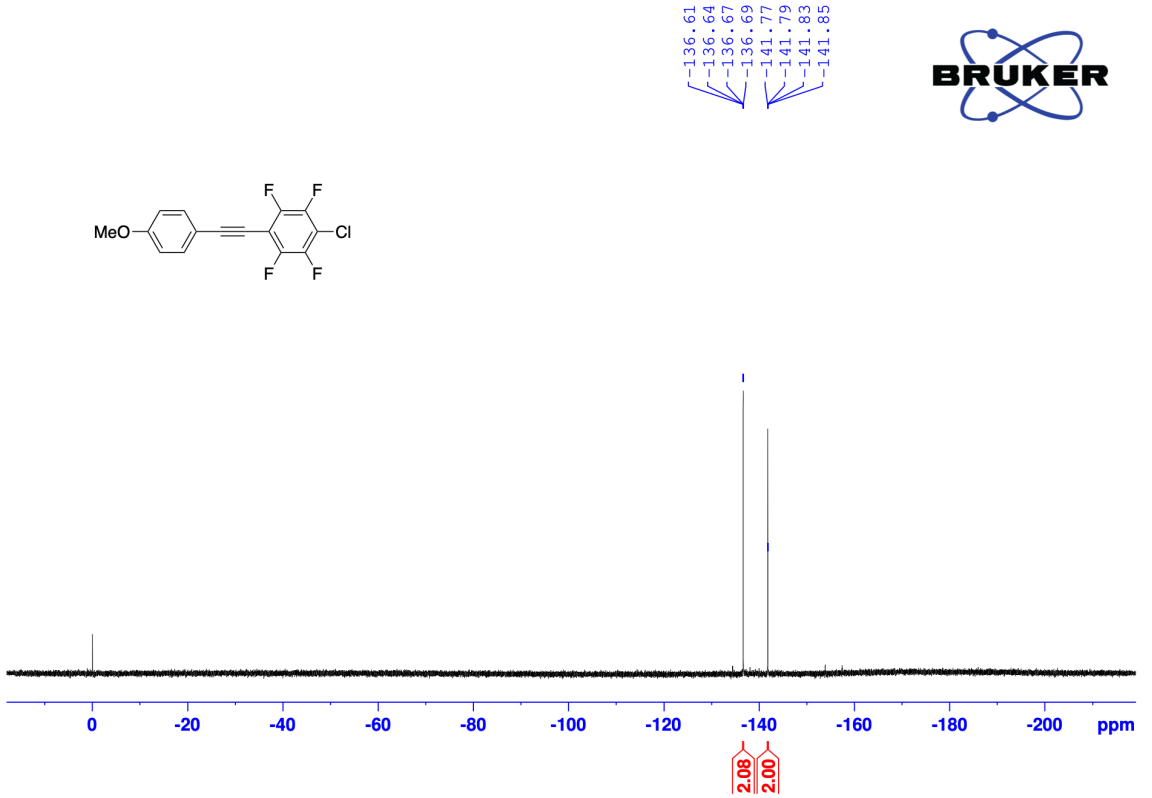



**Figure S3** $^{19}$F NMR spectrum of **4F-Cl**.

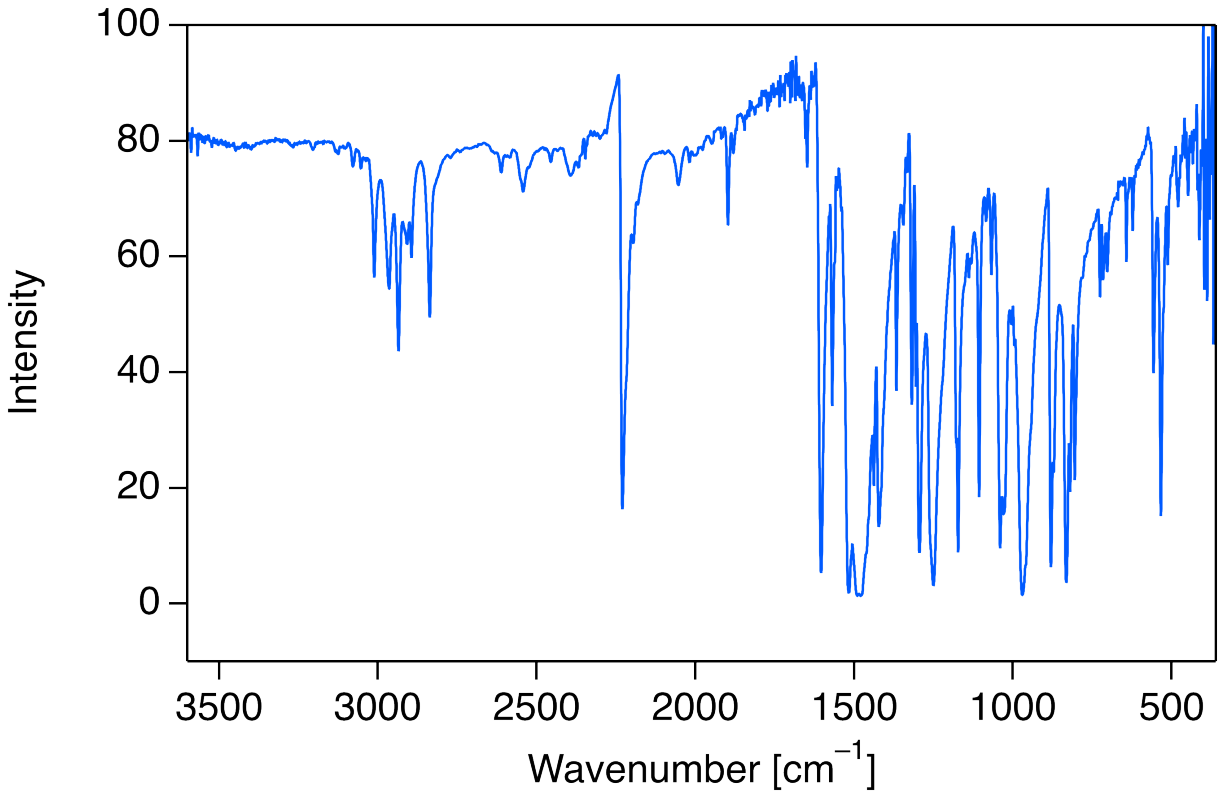



**Figure S4** IR spectrum of **4F-Cl**.

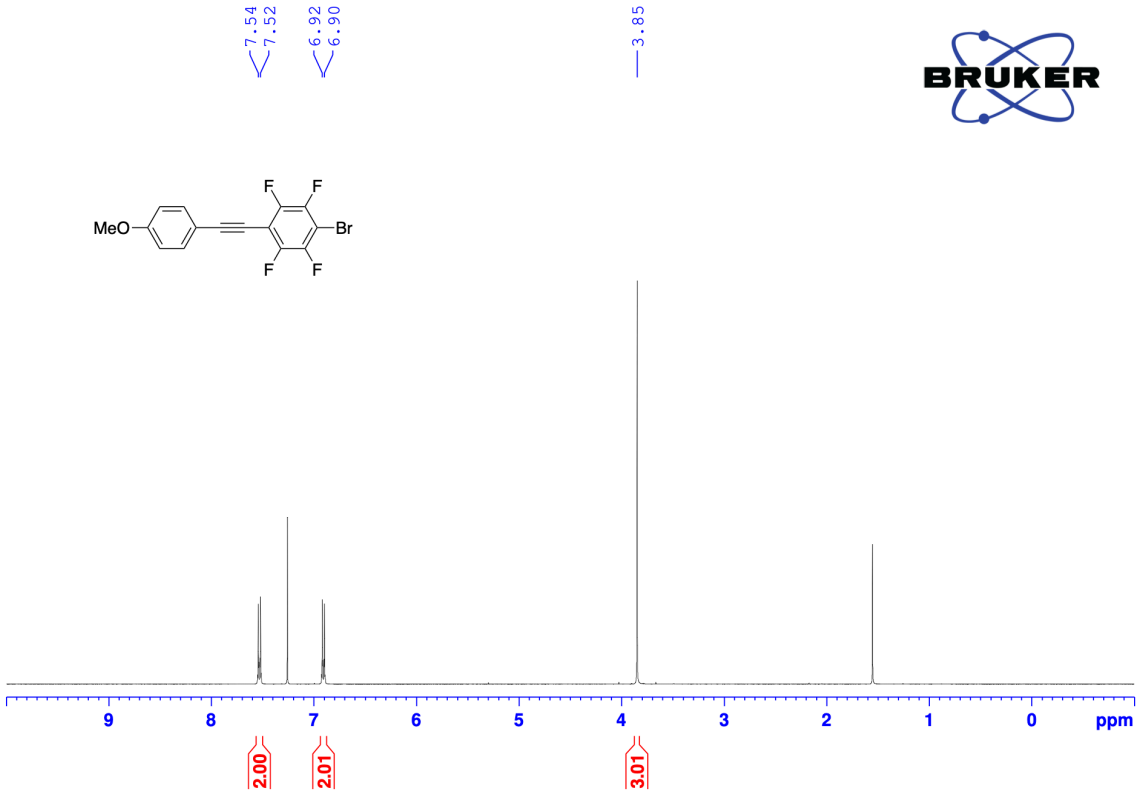



**Figure S5** $^{1}$H NMR spectrum of **4F-Br**.

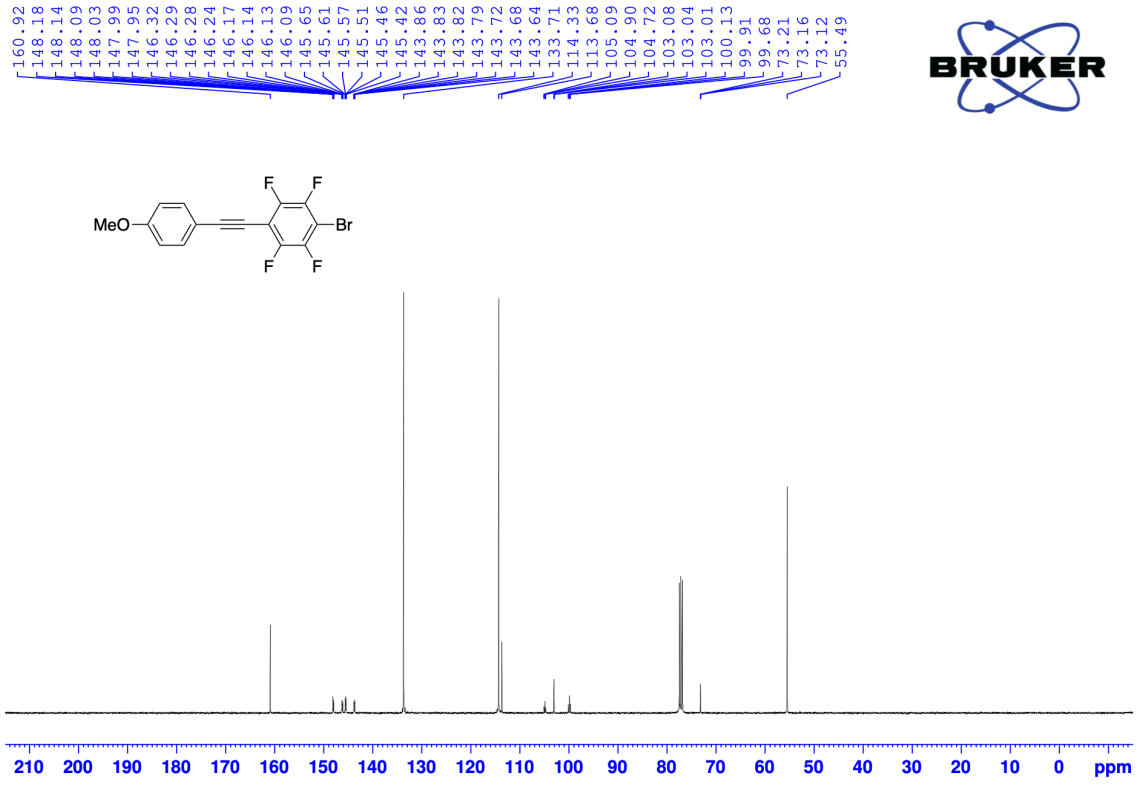



**Figure S6** $^{13}$C NMR spectrum of **4F-Br**.

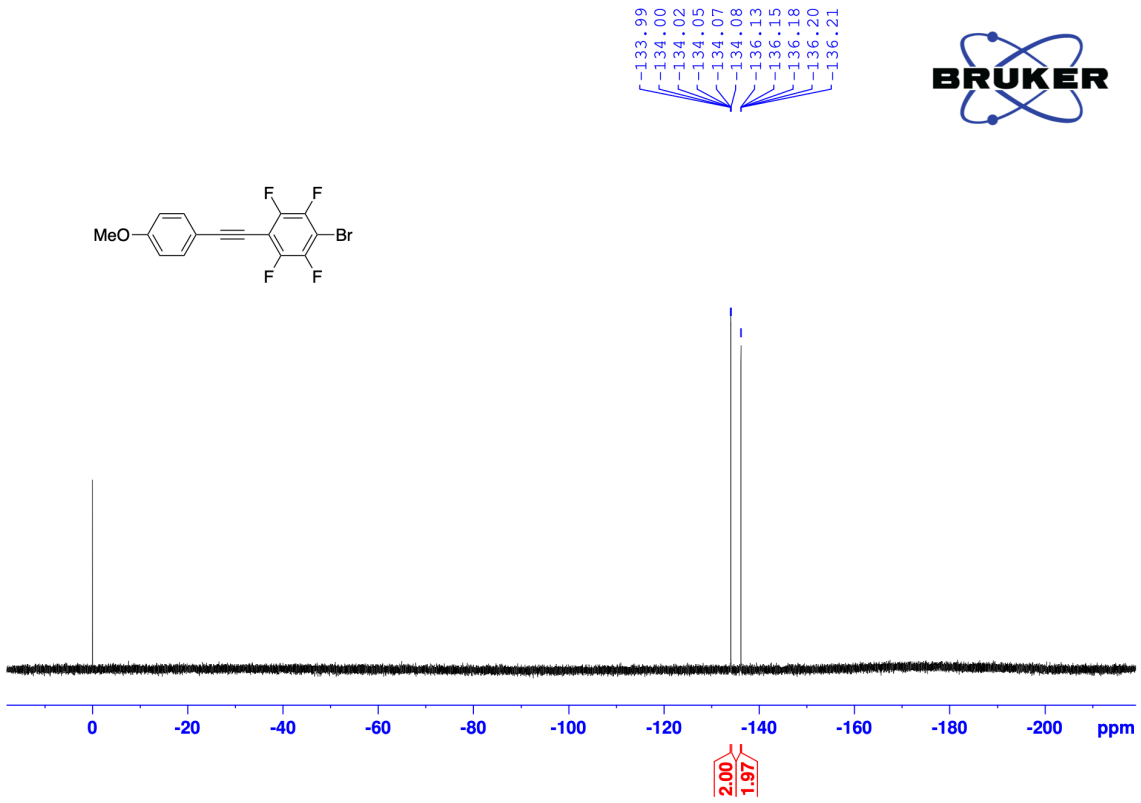



**Figure S7** $^{19}$F NMR spectrum of **4F-Br**.

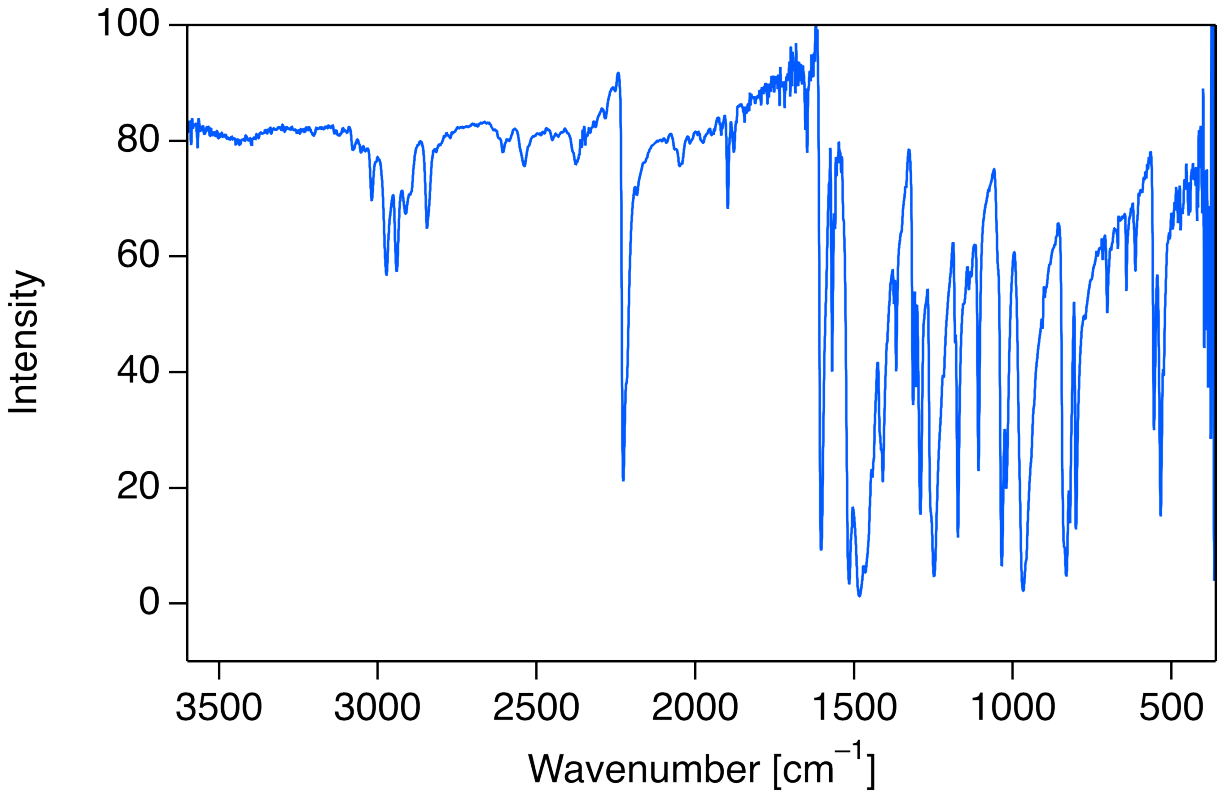



**Figure S8** IR spectrum of **4F-Br**.

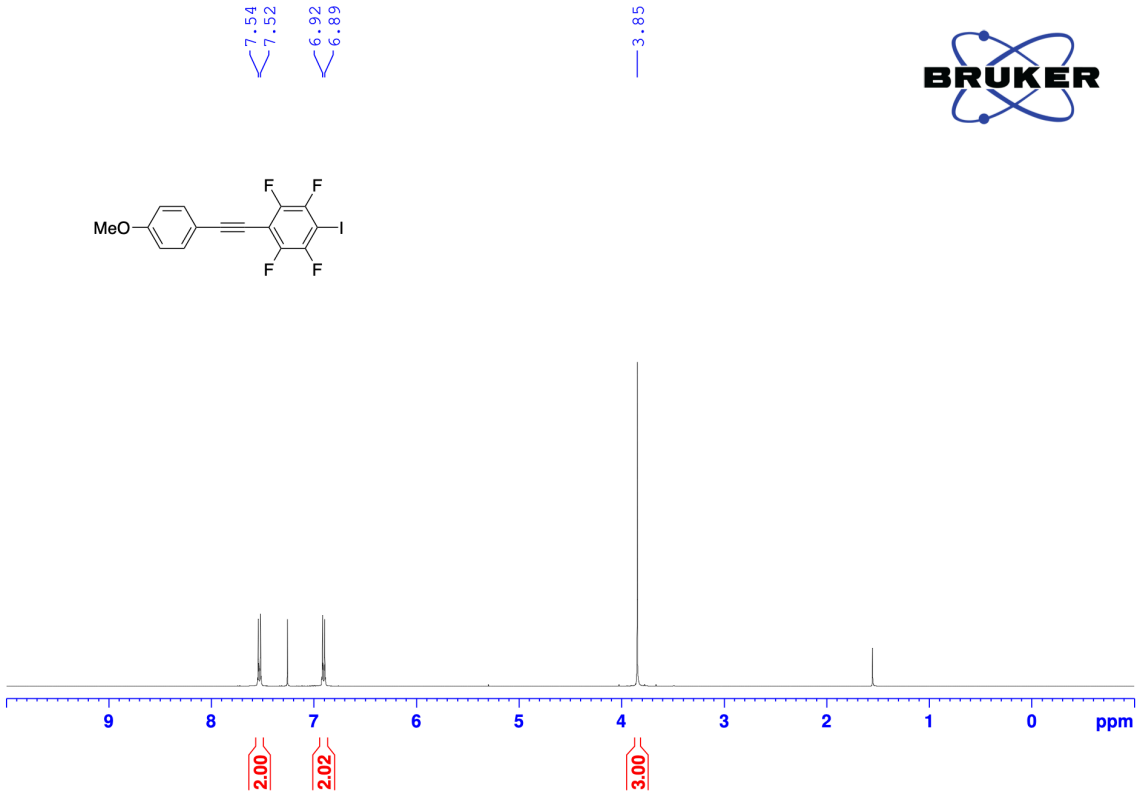



**Figure S9** $^{1}$H NMR spectrum of **4F-I**.

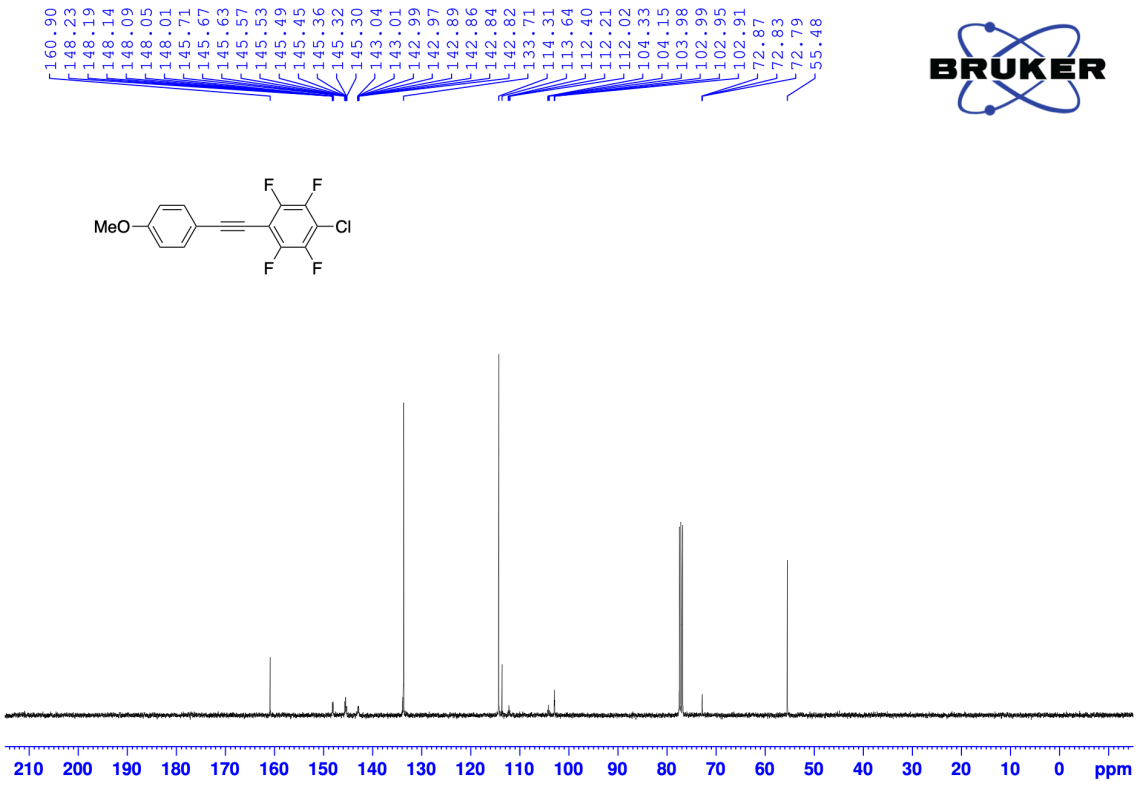



**Figure S10** $^{13}$C NMR spectrum of **4F-I**.

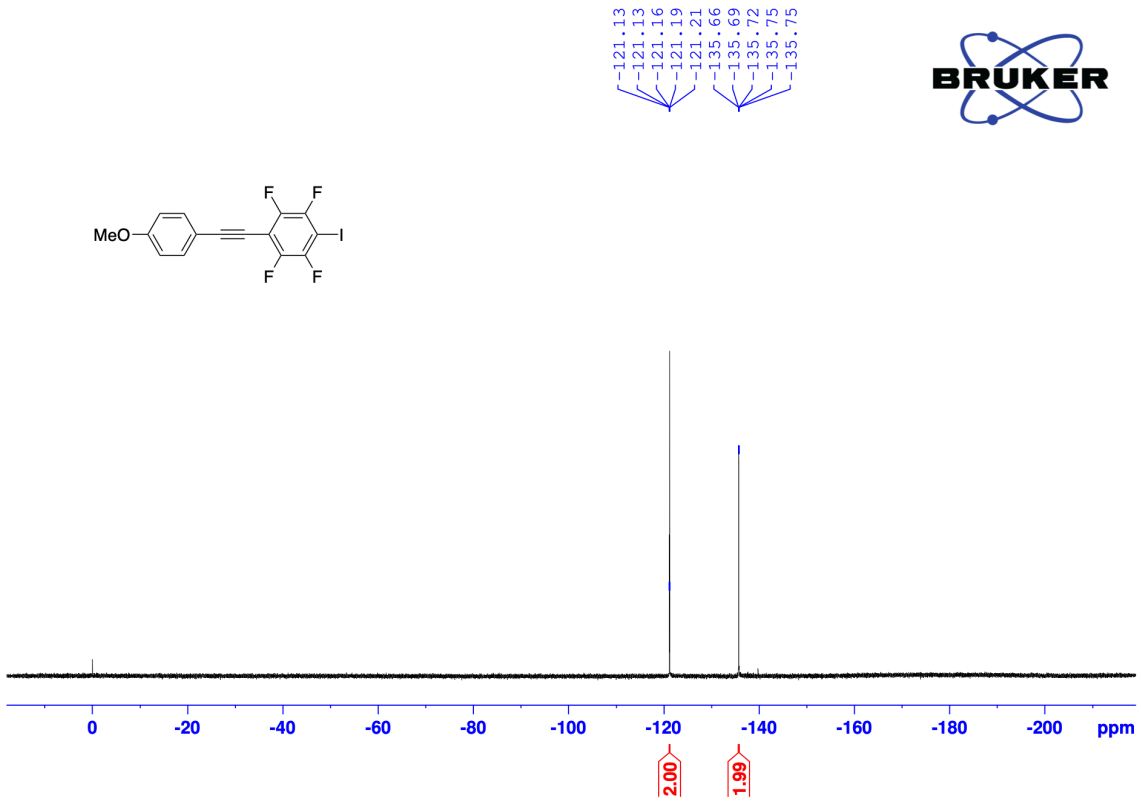



**Figure S11** $^{19}$F NMR spectrum of **4F-I**.

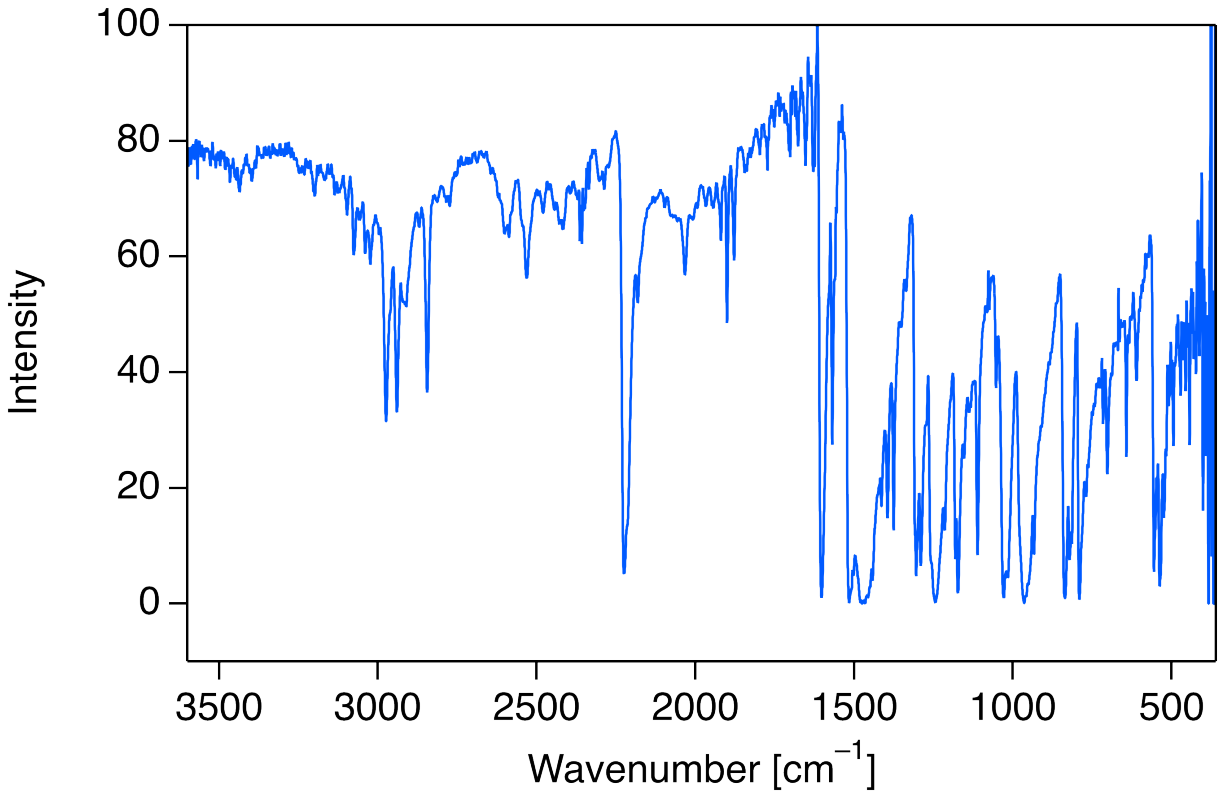



**Figure S12** IR spectrum of **4F-I**.

## 2. Crystallographic data

**Table S1** Crystallographic data of **4F-Cl**, **4F-Br**, and **4F-I**.

| | **4F-Cl** | **4F-Br** | **4F-I** |
|---|---|---|---|
| CCDC # | 2116928 | 2116929 | 2116930 |
| Empirical Formula | $C_{15}H_7ClF_4O$ | $C_{15}H_7BrF_4O$ | $C_{15}H_7F_4IO$ |
| Formula weight | 314.66 | 359.11 | 406.11 |
| Temperature [K] | 299 | 293 | 293 |
| Crystal Color / Habit | Colourless / Plate | Colourless / Block | Colourless / Block |
| Crystal Size [mm] | 0.418 × 0.305 × 0.081 | 0.687 × 0.390 × 0.156 | 0.619 × 0.538 × 0.096 |
| Crystal System | triclinic | monoclinic | orthorhombic |
| Space Group | *P*-1 | $P2_1/c$ | *Pbca* |
| *a* [Å] | 6.2618(3) | 7.5810(5) | 16.2038(6) |
| *b* [Å] | 7.4426(3) | 28.9757(12) | 6.1025(2) |
| *c* [Å] | 29.3159(10) | 6.4309(4) | 28.4996(10) |
| *α* [°] | 90.733(3) | 90 | 90 |
| *β* [°] | 92.011(3) | 100.322(7) | 90 |
| *γ* [°] | 97.051(4) | 90 | 90 |
| *V* [Å$^3$] | 1354.87(10) | 1389.78(14) | 2818.15(17) |
| *Z* | 4 | 4 | 8 |
| $R_1$ [$F^2 > 2\sigma(F^2)$] [a] | 0.0707 | 0.0471 | 0.0342 |
| $wR_2$ ($F^2$) [b] | 0.2402 | 0.1044 | 0.0983 |

[a] $R_1 = \Sigma||F_o| - |F_c|| \,/\, \Sigma|F_o|$. [b] $wR_2 = \{[\Sigma w(|F_o| - |F_c|)]/\Sigma w|F_o|\}^{1/2}$.

## 3. Absorption, PL, PL decay spectra in toluene

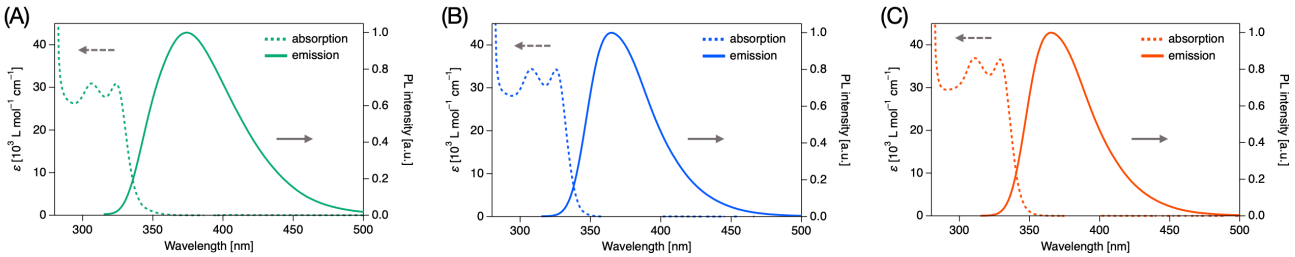



**Figure S13** Absorption (dotted line, left) and PL (solid line, right) spectra of (A) **4F-Cl**, (B) **4F-Br**, and (C) **4F-I** in toluene excited at maximum absorption wavelength.

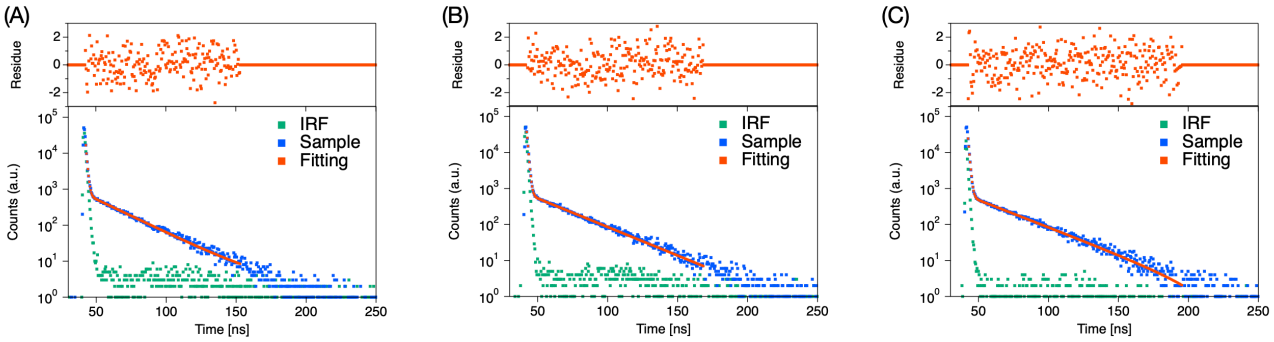



**Figure S14** PL decay profiles monitored at emission maxima of (A) **4F-Cl**, (B) **4F-Br**, and (C) **4F-I** in toluene excited at 280 nm.

## 4. Absorption, PL, and PL decay spectra of in various solvents

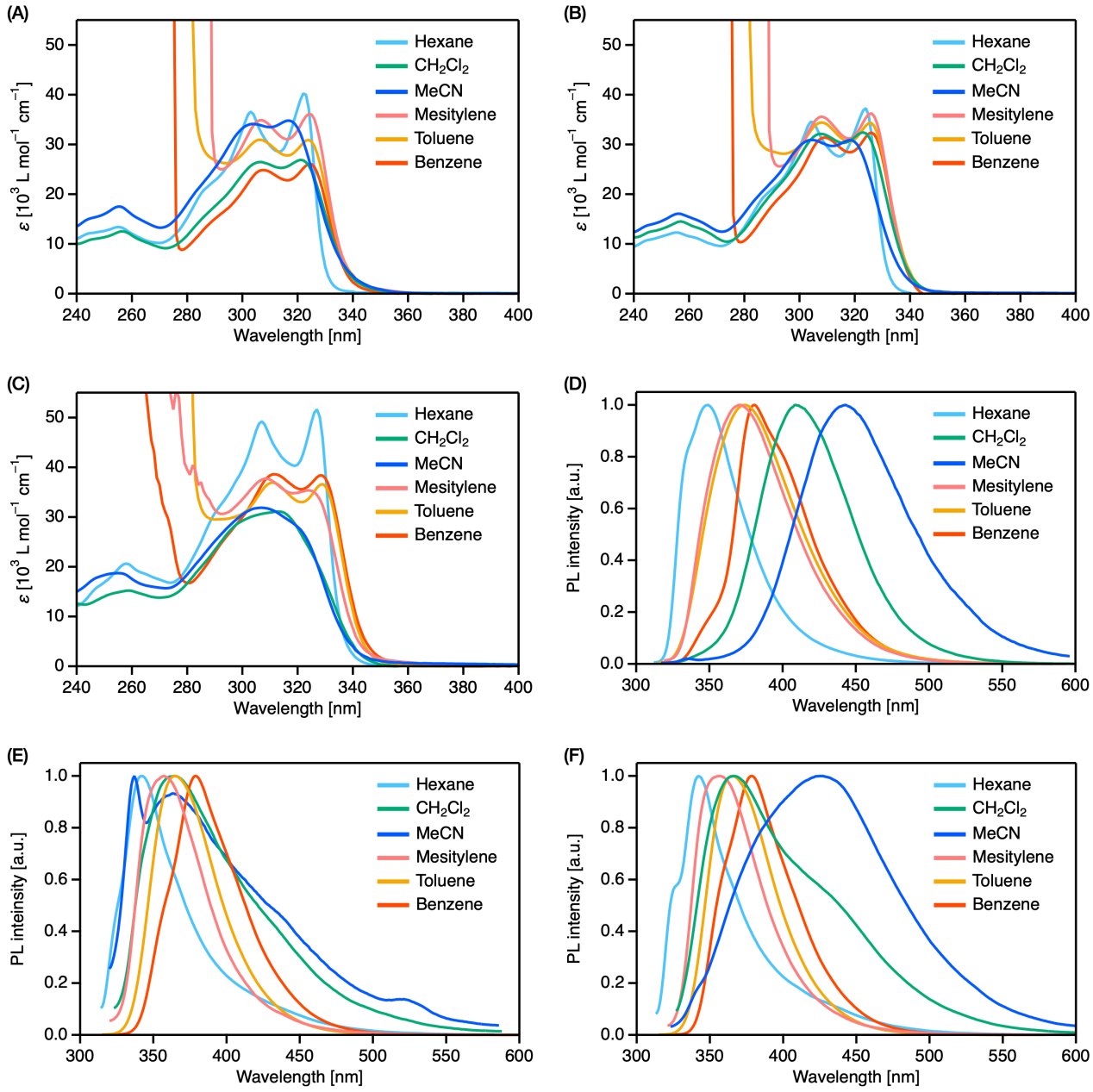



**Figure S15** Absorption spectra of (A) **4F-Cl**, (B) **4F-Br**, (C) **4F-I**, and PL spectra of (D) **4F-Cl**, (E) **4F-Br**, (F) **4F-I** excited at maximum absorption wavelength.

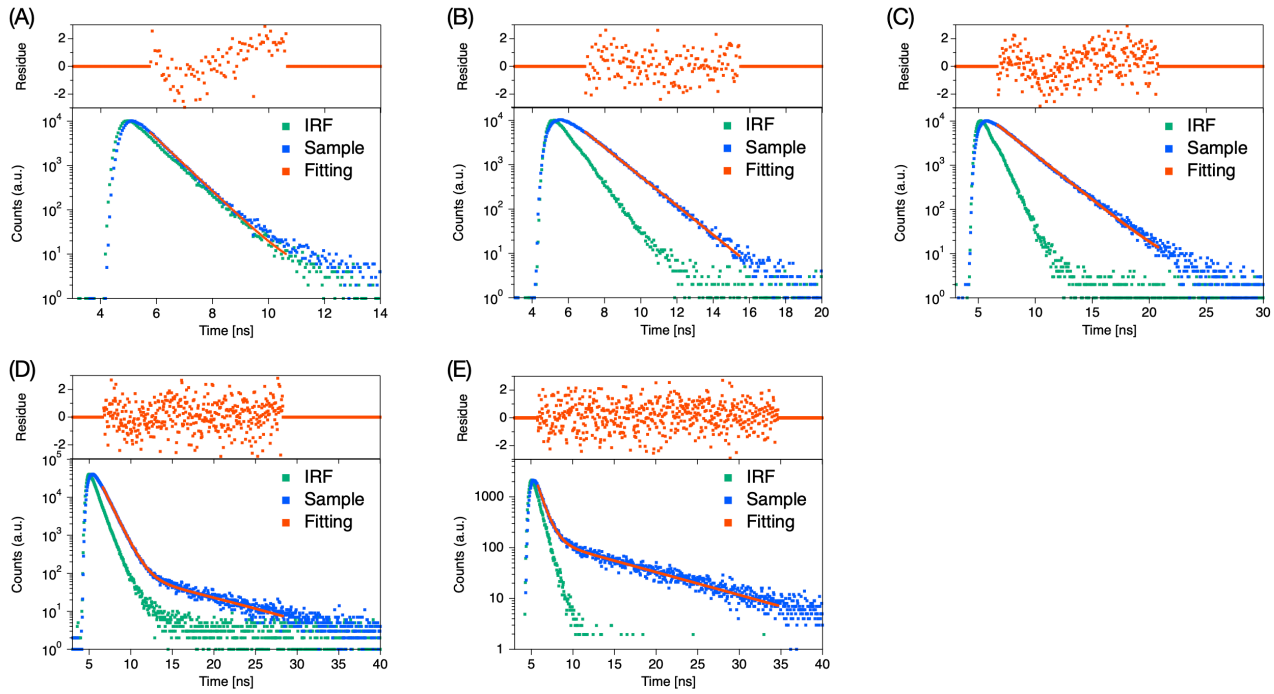



**Figure S16** PL decay profiles monitored at emission maxima of **4F-Cl** in (A) hexane, (B) dichloromethane, (C) acetonitrile, (D) benzene, (E) mesitylene excited at 280 nm.

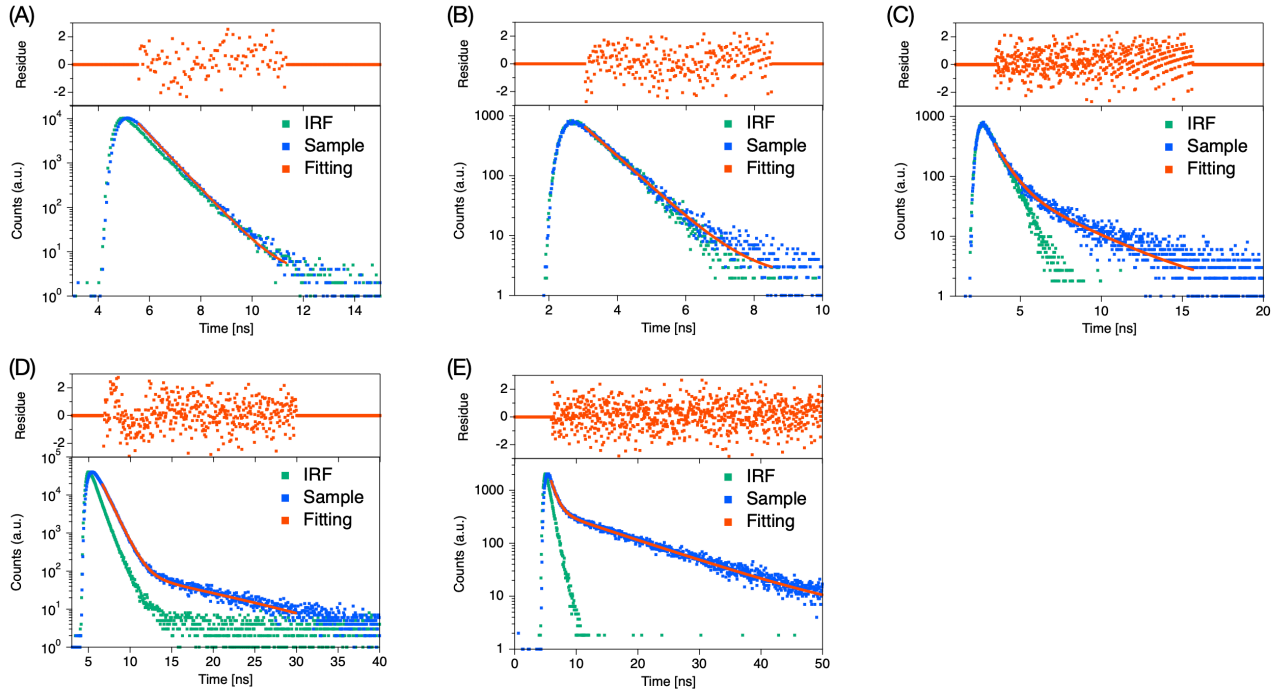



**Figure S17** PL decay profiles monitored at emission maxima of **4F-Br** in (A) hexane, (B) dichloromethane, (C) acetonitrile, (D) benzene, (E) mesitylene excited at 280 nm.

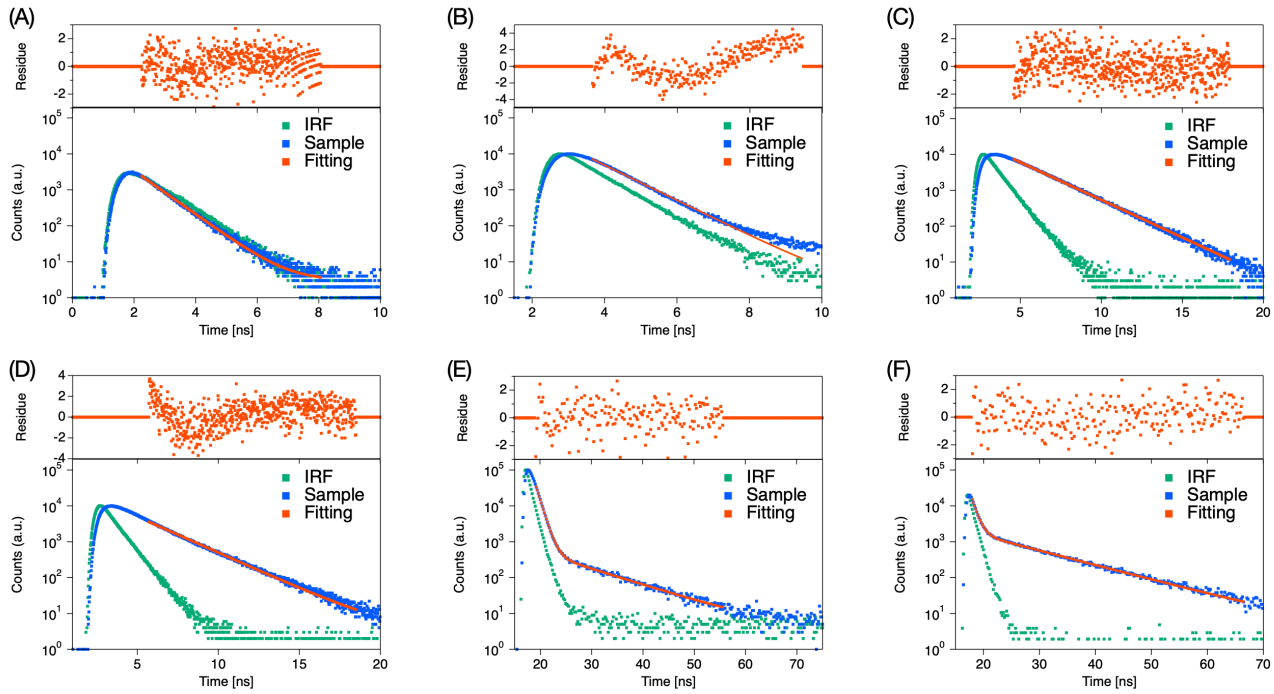



**Figure S18** PL decay profiles monitored at emission maxima of **4F-I** in (A) hexane, (B) THF, (C) dichloromethane, (D) acetonitrile, (E) benzene, (F) mesitylene excited at 280 nm.

**Table S2** Photophysical properties of **4F-Cl** in various solvents.

| Solvents | $\lambda_{max}$ [nm] ($\varepsilon$ [L mol$^{-1}$ cm$^{-1}$]) | $\lambda_{PL}$ [nm] | $\Phi_{PL}$ | $\tau_1$ [ns] | $\tau_2$ [ns] |
|---|---|---|---|---|---|
| Hexane | 303(36600), 322(40200) | 349 | 0.10 | <1.0 | - |
| $CH_2Cl_2$ | 307(26500), 321(26900) | 409 | 0.05 | 1.3 | - |
| MeCN | 304(34100), 317(34800) | 443 | 0.05 | 2.1 | - |
| Mesitylene | 307(34900), 324(36100) | 370 | 0.14 | <1.0 | 9.7 |
| Toluene | 306(30900), 324(30900) | 374 | 0.15 | <1.0 | 23.4 |
| Benzene | 308(24800), 324(26100) | 381 | 0.31 | <1.0 | 8.0 |

**Table S3** Photophysical properties of **4F-Br** in various solvents.

| Solvents | $\lambda_{max}$ [nm] ($\varepsilon$ [L mol$^{-1}$ cm$^{-1}$]) | $\lambda_{PL}$ [nm] | $\Phi_{PL}$ | $\tau_1$ [ns] | $\tau_2$ [ns] |
|---|---|---|---|---|---|
| Hexane | 304(34500), 324(37300) | 342 | 0.01 | <1.0 | - |
| $CH_2Cl_2$ | 308(32100), 323(32400) | 364 | 0.01 | <1.0 | - |
| MeCN | 304(30900), 318(30900) | 337 | 0.01 | <1.0 | 3.3 |
| Mesitylene | 308(35600), 326(36200) | 357 | 0.02 | <1.0 | 11.2 |
| Toluene | 308(34400), 326(34300) | 365 | 0.45 | <1.0 | 23.4 |
| Benzene | 309(31400), 326(32400) | 379 | 0.21 | <1.0 | 9.5 |

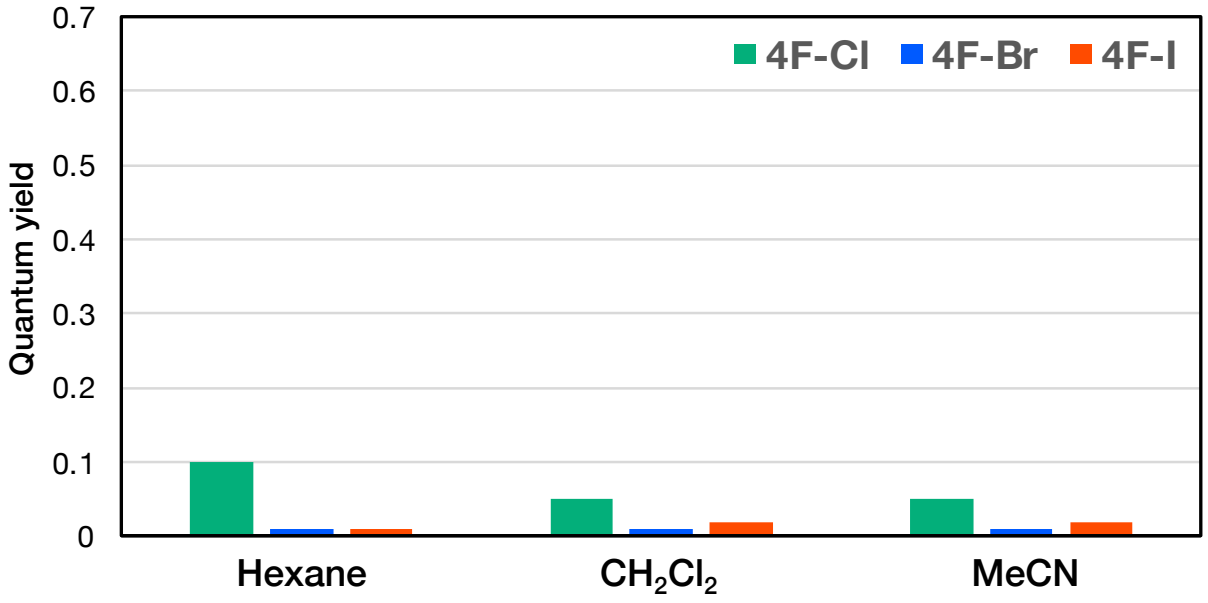



**Figure S19** Relationship between solvents and quantum yields.

## 5. PL and PL decay spectra of crystal

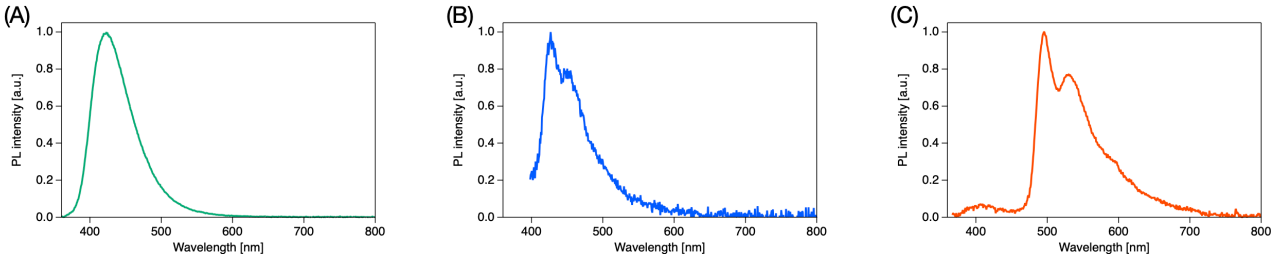



**Figure S20** PL spectra of (A) **4F-Cl**, (B) **4F-Br**, and (C) **4F-I** in crystal excited at 330 nm (**4F-Cl**), 390 nm (**4F-Br**), 350 nm (**4F-I**).

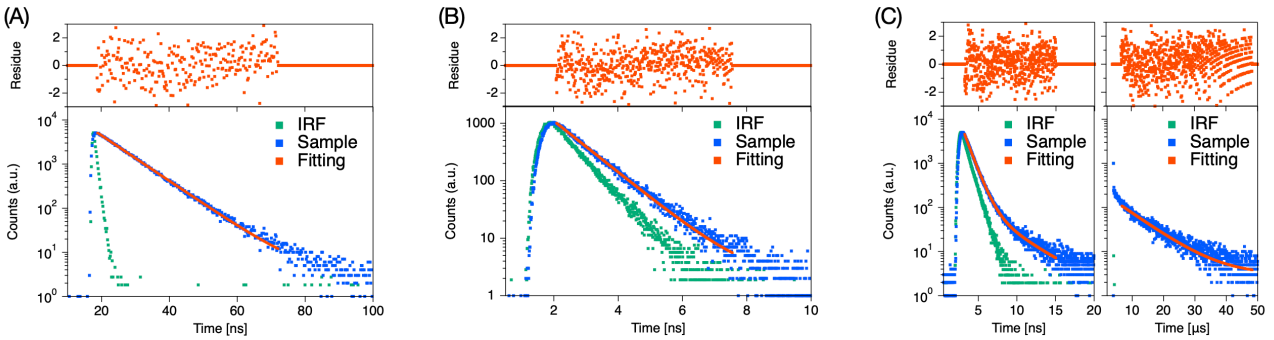



**Figure S21** PL decay profiles monitored at emission maxima of (A) **4F-Cl**, (B) **4F-Br**, (C) **4F-Cl** (monitored wavelength, left; 406 nm, right; 495 nm) excited at 280 nm.

## 6. PL and PL decay spectra of 4F-I in polymer matrix

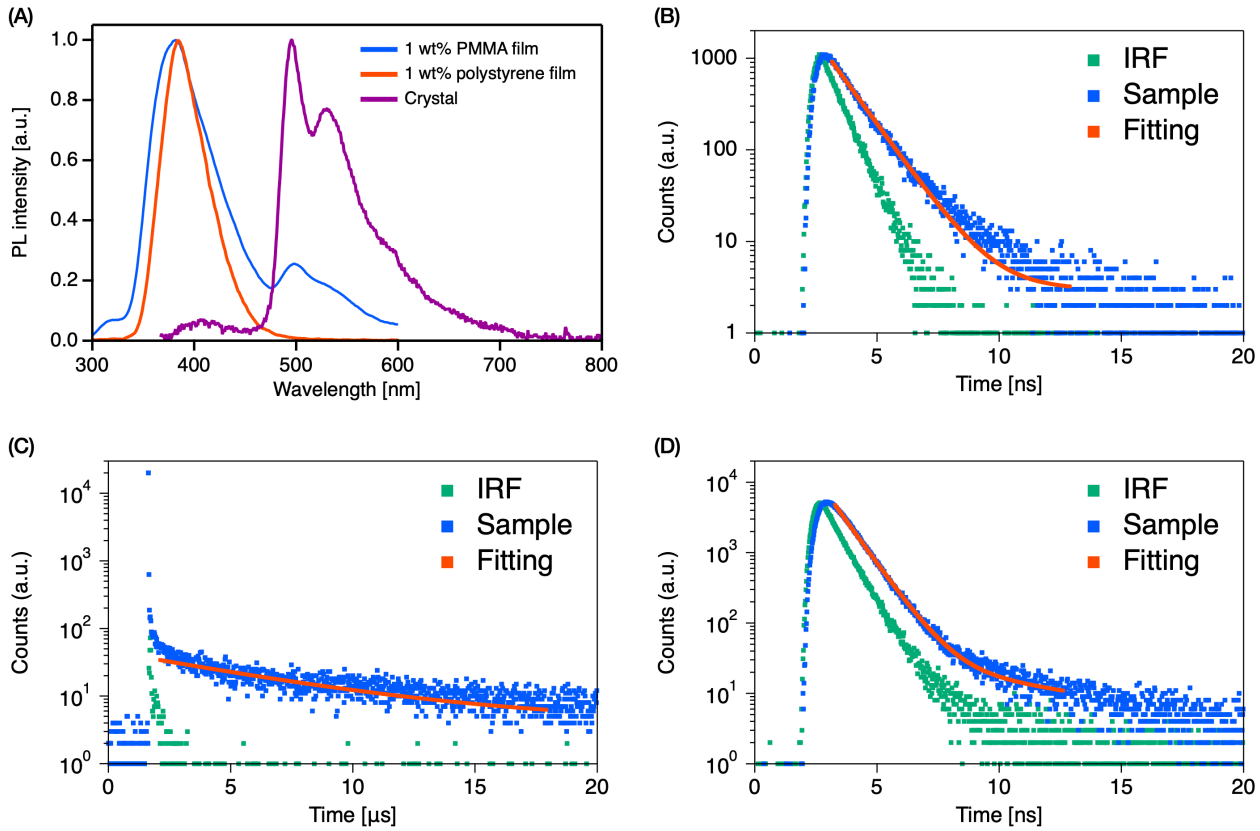



**Figure S22** (A) PL spectra of **4F-I** dispersed in PMMA or polystyrene matrix, PL decay profiles in (B) PMMA (monitored at 382 nm), (C) PMMA (monitored at 498 nm), (D) polystyrene (monitored at 384 nm) excited at 280 nm.

**Table S4** Photophysical properties of **4F-I** in polymer matrix.

| Polymer matrix | $\lambda_{PL}$ [nm] | $\Phi_{PL}$ | Fluorescence | | Phosphorescence |
|---|---|---|---|---|---|
| | | | $\tau_1$ [ns] | $\tau_2$ [ns] | $\tau_{phos}$ [$\mu$s] |
| PMMA | 382, 498 | 0.01 | 1.2 | - | 6.1 |
| Polystyrene | 384 | 0.05 | <1.0 | 10.2 | - |

## 7. Quantum chemical calculation

All computations were carried out using density functional theory (DFT) with the Gaussian 16 (Rev. B.01) package. Geometry optimizations of single molecule were executed using the M06-2X hybrid functional and 6-31+G(d) basis set with a CPCM for toluene. **4F** and benzene were optimized using the M06-2X hybrid functional and 6-31+G(d) basis set. Vertical excitations were also calculated using a TD-DFT method at the same level of theory.

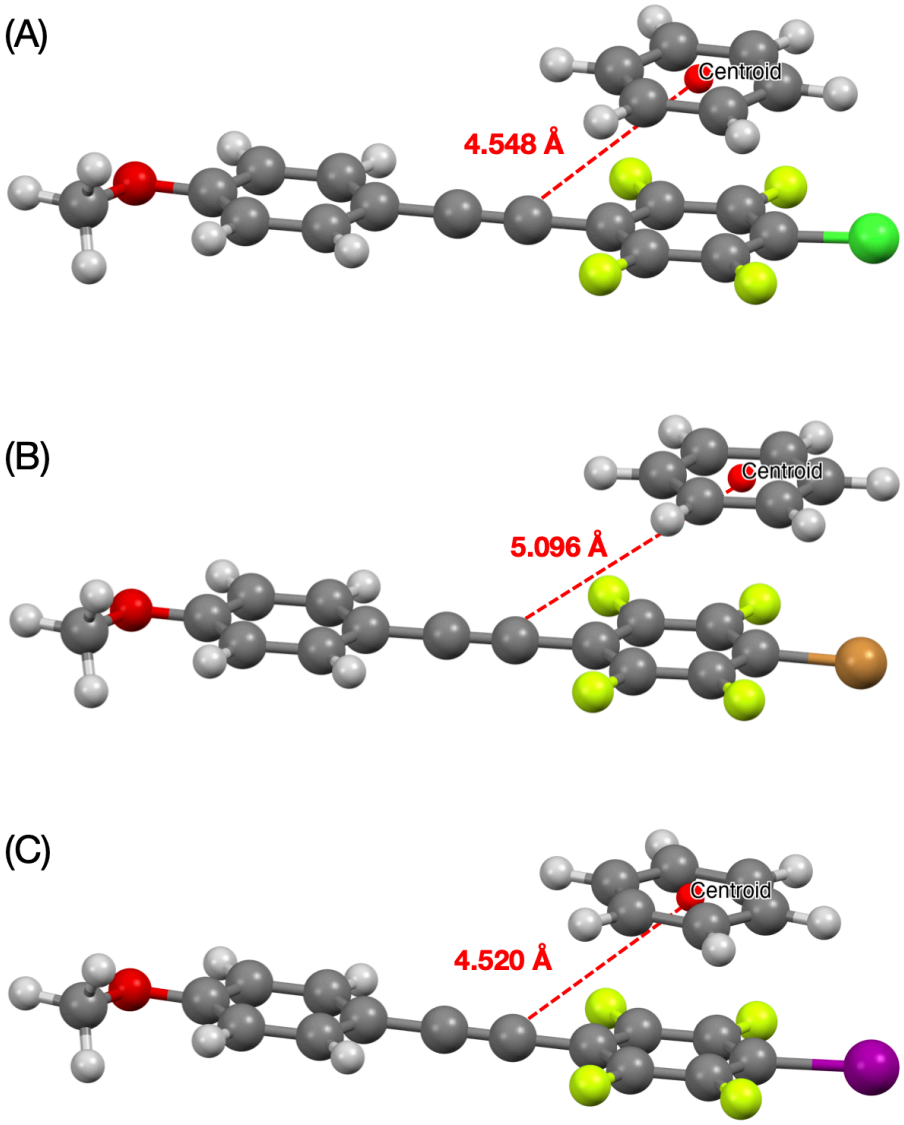
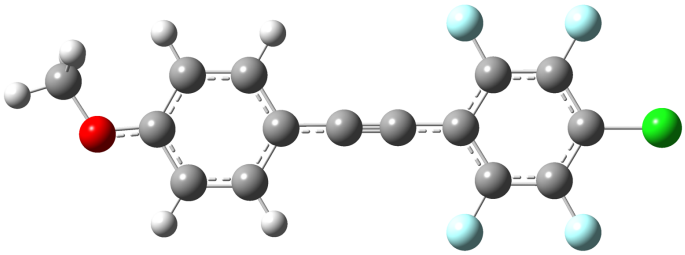



**Figure S23** Optimized structures and the distance between the carbon atom of alkyne and centroid of benzene (A) **4F-Cl**, (B) **4F-Br**, and (C) **4F-I**.

## • Geometry optimization of 4F-Cl



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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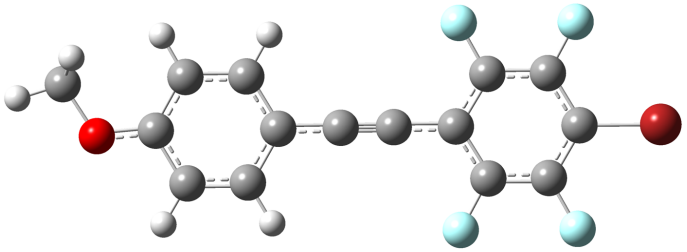
| 2 | 6 | 0 | -3.402124 | 1.372237 | 0.000000 |
| 3 | 6 | 0 | -2.728619 | 0.135734 | 0.000002 |
| 4 | 6 | 0 | -3.480064 | -1.045249 | 0.000004 |
| 5 | 6 | 0 | -4.871904 | -1.008326 | 0.000002 |
| 6 | 6 | 0 | -5.528129 | 0.227245 | 0.000000 |
| 7 | 1 | 0 | -5.315829 | 2.362720 | -0.000004 |
| 8 | 1 | 0 | -2.827700 | 2.293363 | -0.000002 |
| 9 | 1 | 0 | -2.969004 | -2.003100 | 0.000006 |
| 10 | 1 | 0 | -5.426259 | -1.939266 | 0.000003 |
| 11 | 6 | 0 | -1.300572 | 0.088674 | 0.000003 |
| 12 | 6 | 0 | -0.088801 | 0.052197 | 0.000002 |
| 13 | 6 | 0 | 1.331904 | 0.014894 | 0.000002 |
| 14 | 6 | 0 | 2.093444 | 1.188365 | -0.000002 |
| 15 | 6 | 0 | 2.034245 | -1.194869 | 0.000004 |
| 16 | 6 | 0 | 3.478280 | 1.158092 | -0.000003 |
| 17 | 6 | 0 | 3.418964 | -1.233096 | 0.000002 |
| 18 | 6 | 0 | 4.161545 | -0.055200 | -0.000001 |
| 19 | 8 | 0 | -6.873545 | 0.375139 | -0.000002 |
| 20 | 6 | 0 | -7.673127 | -0.796099 | -0.000001 |
| 21 | 1 | 0 | -7.485795 | -1.397565 | -0.896212 |
| 22 | 1 | 0 | -7.485797 | -1.397562 | 0.896213 |
| 23 | 1 | 0 | -8.706226 | -0.451585 | -0.000002 |
| 24 | 9 | 0 | 1.481704 | 2.372616 | -0.000004 |
| 25 | 9 | 0 | 4.153720 | 2.306121 | -0.000007 |
| 26 | 9 | 0 | 1.364585 | -2.347462 | 0.000007 |
| 27 | 9 | 0 | 4.036817 | -2.413226 | 0.000004 |
| 28 | 17 | 0 | 5.876856 | -0.097580 | -0.000004 |

Excited State 1: Singlet-A 4.1041 eV 302.10 nm f=1.4614 <S**2>=0.000

HOMO -> LUMO 0.68706

• **Geometry optimization of 4F-Br**



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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| 3 | 6 | 0 | 3.355890 | 0.137336 | -0.000001 |
| 4 | 6 | 0 | 4.102172 | -1.046856 | -0.000002 |
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| 8 | 1 | 0 | 3.463826 | 2.294545 | 0.000001 |
| 9 | 1 | 0 | 3.586981 | -2.002493 | -0.000003 |
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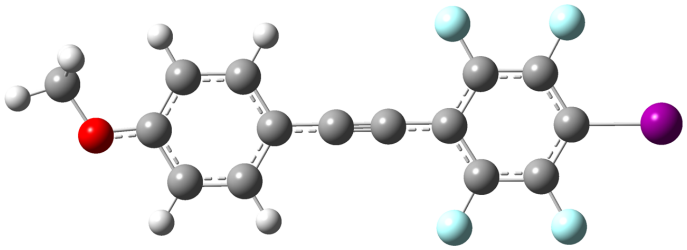
| 11 | 6 | 0 | 1.927977 | 0.096038 | 0.000000 |
| 12 | 6 | 0 | 0.716177 | 0.065189 | 0.000000 |
| 13 | 6 | 0 | -0.704018 | 0.031653 | 0.000001 |
| 14 | 6 | 0 | -1.461791 | 1.207266 | 0.000001 |
| 15 | 6 | 0 | -1.407239 | -1.177455 | 0.000001 |
| 16 | 6 | 0 | -2.846000 | 1.177639 | 0.000001 |
| 17 | 6 | 0 | -2.791362 | -1.211916 | 0.000002 |
| 18 | 6 | 0 | -3.529486 | -0.033403 | 0.000002 |
| 19 | 8 | 0 | 7.501499 | 0.358969 | 0.000000 |
| 20 | 6 | 0 | 8.295593 | -0.815987 | 0.000000 |
| 21 | 1 | 0 | 8.105429 | -1.416569 | 0.896207 |
| 22 | 1 | 0 | 8.105430 | -1.416567 | -0.896208 |
| 23 | 1 | 0 | 9.330296 | -0.476323 | 0.000001 |
| 24 | 9 | 0 | -0.845902 | 2.389243 | 0.000000 |
| 25 | 9 | 0 | -3.517698 | 2.328359 | 0.000000 |
| 26 | 9 | 0 | -0.737728 | -2.330118 | -0.000001 |
| 27 | 9 | 0 | -3.409532 | -2.392228 | 0.000001 |
| 28 | 35 | 0 | -5.387214 | -0.076744 | -0.000001 |

Excited State 1: Singlet-A 4.0786 eV 303.99 nm f=1.5260 <S**2>=0.000

HOMO -> LUMO 0.68703

## • Geometry optimization of 4F-I



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
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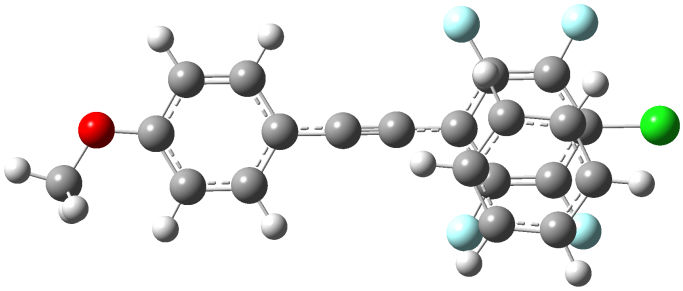
| 3 | 6 | 0 | -3.921645 | 0.137010 | -0.000003 |
| 4 | 6 | 0 | -4.665402 | -1.048962 | 0.000005 |
| 5 | 6 | 0 | -6.057592 | -1.021344 | 0.000005 |
| 6 | 6 | 0 | -6.722201 | 0.209852 | -0.000003 |
| 7 | 1 | 0 | -6.523884 | 2.346616 | -0.000016 |
| 8 | 1 | 0 | -4.035348 | 2.293850 | -0.000015 |
| 9 | 1 | 0 | -4.148001 | -2.003265 | 0.000012 |
| 10 | 1 | 0 | -6.605499 | -1.955967 | 0.000011 |
| 11 | 6 | 0 | -2.493611 | 0.099067 | 0.000001 |
| 12 | 6 | 0 | -1.281686 | 0.069757 | 0.000005 |
| 13 | 6 | 0 | 0.138880 | 0.039234 | -0.000001 |
| 14 | 6 | 0 | 0.895649 | 1.215226 | 0.000005 |
| 15 | 6 | 0 | 0.847106 | -1.166572 | -0.000005 |
| 16 | 6 | 0 | 2.281165 | 1.186875 | 0.000005 |
| 17 | 6 | 0 | 2.232682 | -1.194579 | -0.000005 |
| 18 | 6 | 0 | 2.974090 | -0.018424 | 0.000000 |
| 19 | 8 | 0 | -8.068405 | 0.348586 | -0.000003 |
| 20 | 6 | 0 | -8.859641 | -0.827800 | 0.000010 |
| 21 | 1 | 0 | -8.668227 | -1.428232 | -0.896088 |
| 22 | 1 | 0 | -8.668218 | -1.428218 | 0.896115 |
| 23 | 1 | 0 | -9.895242 | -0.490833 | 0.000012 |
| 24 | 9 | 0 | 0.278716 | 2.397132 | 0.000011 |
| 25 | 9 | 0 | 2.939574 | 2.347518 | 0.000010 |
| 26 | 9 | 0 | 0.182557 | -2.322508 | -0.000008 |
| 27 | 9 | 0 | 2.843267 | -2.381234 | -0.000009 |
| 28 | 53 | 0 | 5.060820 | -0.060508 | -0.000001 |

Excited State 1: Singlet-A 4.0848 eV 303.52 nm f=1.5789 <S**2>=0.000

HOMO -> LUMO 0.68784

## • Geometry optimization of 4F-Cl and benzene

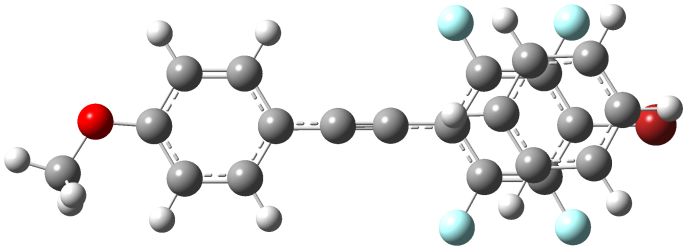


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.484423 | 1.212795 | 0.757061 |
| 2 | 6 | 0 | -4.112214 | 1.323847 | 0.633937 |
| 3 | 6 | 0 | -3.386147 | 0.393272 | -0.133103 |
| 4 | 6 | 0 | -4.077175 | -0.644199 | -0.768084 |
| 5 | 6 | 0 | -5.459500 | -0.762824 | -0.648981 |
| 6 | 6 | 0 | -6.167385 | 0.168802 | 0.116442 |
| 7 | 1 | 0 | -6.058512 | 1.922106 | 1.344283 |
| 8 | 1 | 0 | -3.583276 | 2.132296 | 1.129008 |
| 9 | 1 | 0 | -3.524114 | -1.364882 | -1.362654 |
| 10 | 1 | 0 | -5.966906 | -1.576888 | -1.153078 |
| 11 | 6 | 0 | -1.967630 | 0.507202 | -0.261401 |
| 12 | 6 | 0 | -0.764541 | 0.605998 | -0.369626 |
| 13 | 6 | 0 | 0.647141 | 0.714692 | -0.491679 |
| 14 | 6 | 0 | 1.358826 | 1.739792 | 0.138342 |
| 15 | 6 | 0 | 1.389447 | -0.224019 | -1.216183 |
| 16 | 6 | 0 | 2.739311 | 1.821756 | 0.057139 |
| 17 | 6 | 0 | 2.769523 | -0.148400 | -1.303486 |
| 18 | 6 | 0 | 3.462343 | 0.876821 | -0.664731 |
| 19 | 8 | 0 | -7.509603 | 0.146141 | 0.297334 |
| 20 | 6 | 0 | -8.246776 | -0.885450 | -0.328438 |
| 21 | 1 | 0 | -8.140522 | -0.839614 | -1.418632 |
| 22 | 1 | 0 | -7.928960 | -1.870864 | 0.031995 |
| 23 | 1 | 0 | -9.287941 | -0.716196 | -0.056219 |
| 24 | 9 | 0 | 0.706094 | 2.653723 | 0.857047 |
| 25 | 9 | 0 | 3.372757 | 2.804645 | 0.696153 |
| 26 | 9 | 0 | 0.764177 | -1.226308 | -1.831442 |
| 27 | 9 | 0 | 3.431023 | -1.069122 | -2.000628 |
| 28 | 6 | 0 | 1.711853 | -2.924415 | 0.755732 |
| 29 | 6 | 0 | 1.138557 | -1.959883 | 1.584284 |
| 30 | 6 | 0 | 1.948633 | -1.024207 | 2.229544 |
| 31 | 6 | 0 | 3.331584 | -1.055971 | 2.048245 |
| 32 | 6 | 0 | 3.905149 | -2.022442 | 1.220669 |
| 33 | 6 | 0 | 3.094962 | -2.955212 | 0.573522 |
| 34 | 1 | 0 | 1.080240 | -3.644248 | 0.243289 |
| 35 | 1 | 0 | 0.060281 | -1.926644 | 1.715978 |
| 36 | 1 | 0 | 1.500404 | -0.268144 | 2.869159 |
| 37 | 1 | 0 | 3.962766 | -0.322837 | 2.544443 |
| 38 | 1 | 0 | 4.981299 | -2.040660 | 1.072142 |
| 39 | 1 | 0 | 3.540244 | -3.699042 | -0.080774 |
| 40 | 17 | 0 | 5.175655 | 0.943078 | -0.724883 |

Excited State 1: Singlet-A 4.2411 eV 292.34 nm f=1.1705 <S**2>=0.000

HOMO -> LUMO 0.68730

## • Geometry optimization of 4F-Br and benzene

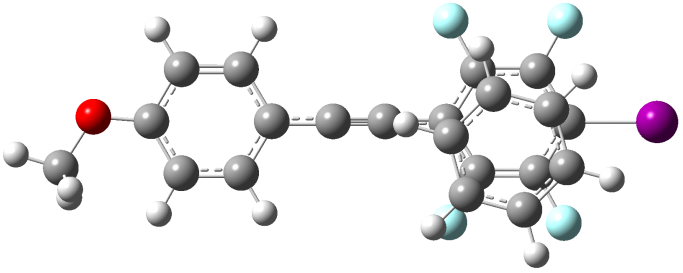


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.056547 | -1.350798 | 0.398535 |
| 2 | 6 | 0 | 4.682787 | -1.365306 | 0.247228 |
| 3 | 6 | 0 | 4.002019 | -0.219731 | -0.206205 |
| 4 | 6 | 0 | 4.739298 | 0.931759 | -0.501755 |
| 5 | 6 | 0 | 6.123439 | 0.954447 | -0.351425 |
| 6 | 6 | 0 | 6.786094 | -0.190790 | 0.100462 |
| 7 | 1 | 0 | 6.596269 | -2.225430 | 0.746715 |
| 8 | 1 | 0 | 4.117493 | -2.262958 | 0.477727 |
| 9 | 1 | 0 | 4.221124 | 1.818915 | -0.852655 |
| 10 | 1 | 0 | 6.667307 | 1.861361 | -0.588051 |
| 11 | 6 | 0 | 2.581739 | -0.233028 | -0.358967 |
| 12 | 6 | 0 | 1.376362 | -0.247241 | -0.482896 |
| 13 | 6 | 0 | -0.037354 | -0.259135 | -0.625387 |
| 14 | 6 | 0 | -0.794794 | -1.388190 | -0.298380 |
| 15 | 6 | 0 | -0.736875 | 0.871673 | -1.058521 |
| 16 | 6 | 0 | -2.174296 | -1.394369 | -0.413993 |
| 17 | 6 | 0 | -2.116408 | 0.871247 | -1.173693 |
| 18 | 6 | 0 | -2.852182 | -0.265310 | -0.858534 |
| 19 | 8 | 0 | 8.125899 | -0.276430 | 0.280648 |
| 20 | 6 | 0 | 8.909442 | 0.863590 | -0.011754 |
| 21 | 1 | 0 | 8.812776 | 1.147803 | -1.066179 |
| 22 | 1 | 0 | 8.626958 | 1.709667 | 0.625684 |
| 23 | 1 | 0 | 9.940281 | 0.579035 | 0.196086 |
| 24 | 9 | 0 | -0.185358 | -2.484513 | 0.153675 |
| 25 | 9 | 0 | -2.845337 | -2.496373 | -0.084437 |
| 26 | 9 | 0 | -0.070680 | 1.989292 | -1.350845 |
| 27 | 9 | 0 | -2.731012 | 1.978216 | -1.586117 |
| 28 | 6 | 0 | -2.080561 | 1.966293 | 1.952789 |
| 29 | 6 | 0 | -1.381087 | 0.840715 | 2.390361 |
| 30 | 6 | 0 | -2.073550 | -0.323516 | 2.725613 |
| 31 | 6 | 0 | -3.464225 | -0.364327 | 2.618570 |
| 32 | 6 | 0 | -4.161752 | 0.761657 | 2.181621 |
| 33 | 6 | 0 | -3.471106 | 1.926426 | 1.846473 |
| 34 | 1 | 0 | -1.540918 | 2.871327 | 1.685732 |
| 35 | 1 | 0 | -0.296810 | 0.868529 | 2.463475 |
| 36 | 1 | 0 | -1.528377 | -1.201861 | 3.061650 |
| 37 | 1 | 0 | -4.002235 | -1.273967 | 2.870356 |
| 38 | 1 | 0 | -5.243546 | 0.727542 | 2.090166 |
| 39 | 1 | 0 | -4.014575 | 2.799910 | 1.497380 |
| 40 | 35 | 0 | -4.695791 | -0.297270 | -1.096132 |

Excited State 1: Singlet-A 4.2271 eV 293.31 nm f=1.2632 <S**2>=0.000

HOMO -> LUMO 0.68679

## • Geometry optimization of 4F-I and benzene



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.318385 | -1.289798 | 0.771223 |
| 2 | 6 | 0 | 4.939208 | -1.346804 | 0.697590 |
| 3 | 6 | 0 | 4.230378 | -0.454773 | -0.129213 |
| 4 | 6 | 0 | 4.945870 | 0.488723 | -0.874450 |
| 5 | 6 | 0 | 6.335361 | 0.552222 | -0.806032 |
| 6 | 6 | 0 | 7.025916 | -0.339907 | 0.020042 |
| 7 | 1 | 0 | 6.879255 | -1.970239 | 1.403439 |
| 8 | 1 | 0 | 4.391435 | -2.082519 | 1.278005 |
| 9 | 1 | 0 | 4.406231 | 1.178939 | -1.515448 |
| 10 | 1 | 0 | 6.861414 | 1.293698 | -1.395559 |
| 11 | 6 | 0 | 2.805076 | -0.511835 | -0.206115 |
| 12 | 6 | 0 | 1.595833 | -0.560517 | -0.270084 |
| 13 | 6 | 0 | 0.177719 | -0.607636 | -0.343008 |
| 14 | 6 | 0 | -0.562236 | -1.549625 | 0.376861 |
| 15 | 6 | 0 | -0.541287 | 0.312015 | -1.113062 |
| 16 | 6 | 0 | -1.947625 | -1.567063 | 0.335659 |
| 17 | 6 | 0 | -1.926037 | 0.295899 | -1.154703 |
| 18 | 6 | 0 | -2.649948 | -0.644335 | -0.429903 |
| 19 | 8 | 0 | 8.372773 | -0.364067 | 0.160144 |
| 20 | 6 | 0 | 9.133783 | 0.571929 | -0.576572 |
| 21 | 1 | 0 | 8.990707 | 0.434523 | -1.654867 |
| 22 | 1 | 0 | 8.871346 | 1.599402 | -0.298146 |
| 23 | 1 | 0 | 10.174878 | 0.379506 | -0.319814 |
| 24 | 9 | 0 | 0.068289 | -2.442201 | 1.140994 |
| 25 | 9 | 0 | -2.595183 | -2.477280 | 1.065866 |
| 26 | 9 | 0 | 0.111523 | 1.236166 | -1.816230 |
| 27 | 9 | 0 | -2.552141 | 1.206646 | -1.899925 |
| 28 | 53 | 0 | -4.733981 | -0.615364 | -0.429978 |
| 29 | 6 | 0 | -1.809223 | 3.287408 | 0.495811 |
| 30 | 6 | 0 | -0.464658 | 3.046745 | 0.781342 |
| 31 | 6 | 0 | -0.113072 | 2.066652 | 1.709690 |
| 32 | 6 | 0 | -1.106752 | 1.326538 | 2.352379 |
| 33 | 6 | 0 | -2.451131 | 1.569639 | 2.069214 |
| 34 | 6 | 0 | -2.802662 | 2.550929 | 1.141209 |
| 35 | 1 | 0 | -2.082557 | 4.041789 | -0.236101 |
| 36 | 1 | 0 | 0.308938 | 3.613087 | 0.271128 |
| 37 | 1 | 0 | 0.934230 | 1.869399 | 1.921948 |
| 38 | 1 | 0 | -0.832335 | 0.558570 | 3.070840 |
| 39 | 1 | 0 | -3.225217 | 0.989660 | 2.565554 |
| 40 | 1 | 0 | -3.849314 | 2.732607 | 0.913104 |

Excited State 1: Singlet-A 4.2106 eV 294.46 nm f=1.2375 <S**2>=0.000

HOMO -> LUMO 0.68444